Original scientific paper
Journal of Central European Agriculture, 2019, 20(1), p.504-523

DOI: /10.5513/JCEA01/20.1.2158

Hyperspectral sensing of soil pH, total carbon and total nitrogen content based on linear and non-linear calibration methods

Određivanje pH tla, ukupnog ugljika i dušika u tlu primjenom linearnih i nelinearnih kalibracijskih modela na temelju hiperspektralne refleksije tla

Ivana ŠESTAK[1]*, Lea MIHALJEVSKI BOLTEK[2], Milan MESIĆ[1], Željka ZGORELEC[1] and Aleksandra PERČIN[1]

[1]University of Zagreb, Faculty of Agriculture, Department of General Agronomy, Svetošimunska cesta 25, 10000 Zagreb, Croatia, *correspondence: isestak@agr.hr

[2]University of Zagreb, Faculty of Agriculture, Undergraduate study program: Agroecology, Svetošimunska cesta 25, 10000 Zagreb, Croatia

Abstract

Soil properties can be estimated non-destructively by visible and near infrared (VNIR) reflectance spectroscopy. However, results of calibration models differ in dependence of measurement precision, spectral range, variability of soil properties and calibration methods used for prediction. The objective of research was to estimate the ability of hyperspectral VNIR sensing for field-scale prediction of soil pH, total carbon (TC, %) and total nitrogen (TN, %) content in arable Stagnosols. Total of 200 soil samples taken from field experiment (soil depth: 30 cm; sampling grid: 15x15 m; 2016) was scanned in laboratory using portable spectroradiometer (FieldSpec®3, 350-1,050 nm). Partial least squares regression (PLSR) and artificial neural networks (ANN) were used to build prediction models of selected soil properties based on VNIR spectra ($P<0.05$). Very strong to complete correlation and low root mean squared error was obtained between predicted and measured values for the calibration and validation dataset, and both prediction methods (PLSR validation: TC, %: R^2=0.85, RMSE=0.163; TN, %: R^2=0.76, RMSE=0.018; soil pH: R^2=0.69, RMSE=0.55; ANN validation: TC, %: R^2=0.88, RMSE=0.108; TN, %: R^2=0.86, RMSE=0.012; soil pH: R^2=0.74, RMSE=0.42). ANN models were more efficient in capturing the complex link between selected soil properties and soil reflectance spectra than PLSR. Calibrations defined in this research should help to support site-specific soil survey as addition to standard laboratory analysis.

Keywords: neural networks, partial least squares regression, reflectance spectroscopy, soil carbon and nitrogen content, soil pH

Sažetak

Svojstva tla mogu se procijeniti nedestruktivno mjerenjem refleksije tla u vidljivom i blisko infracrvenom području spektra (eng. VNIR). Međutim, rezultati kalibracijskih modela mogu se razlikovati ovisno o preciznosti mjerenja, spektralnom rasponu, varijabilnosti pedoloških značajki i tipu kalibracijskih metoda primijenjenih u predikciji. Cilj istraživanja bio je procijeniti mogućnosti hiperspektralne VNIR spektroskopije za određivanje pH vrijednosti, sadržaja ukupnog ugljika (TC, %) i ukupnog dušika (TN, %) u obradivom tlu tipa Stagnosols na razini poljskog pokusa. Ukupno 200 uzoraka tla (dubina: 30 cm; mreža uzorkovanja: 15x15 m; 2016.) skenirano je u laboratorijskim uvjetima prijenosnim spektroradiometrom (FieldSpec®3, 350-1050 nm). Multivarijatne statističke metode, parcijalna regresija najmanjih kvadrata (eng. PLSR) i neuralne mreže (eng. ANN), korištene su za izračun predikcijskih modela odabranih pedoloških svojstava na temelju VNIR spektra ($P<0.05$). Između predviđenih i referentnih vrijednosti za kalibracijski i validacijski set podataka, te obje predikcijske metode utvrđena je vrlo jaka do potpuna korelacija i niska korjenovana srednja kvadratna pogreška (PLSR validacija: TC, %: R^2=0.85, RMSE=0.163; TN, %: R^2=0.76, RMSE=0.018; soil pH: R^2=0.69, RMSE=0.55; ANN validacija: TC, %: R^2=0.88, RMSE=0.108; TN, %: R^2=0.86, RMSE=0.012; soil pH: R^2=0.74, RMSE=0.42). ANN modeli učinkovitije su izdvojili kompleksnu vezu između svojstava tla i spektralne refleksije tla u usporedbi s metodom PLSR. Kalibracije definirane ovim istraživanjem predstavljaju potporu preciznim pedološkim istraživanjima kao relevantan alat uz bok standardnim laboratorijskim analizama.

Ključne riječi: hiperspektralna refleksija, neuralne mreže, parcijalna regresija najmanjih kvadrata, pH tla, sadržaj ugljika i dušika u tlu

Introduction

Regarding dynamic composition of soil on the one hand and site-fixed and specific character of the pedosphere, on the other hand, there is a need to direct soil survey for real-time assessment of soil variability. Soil is a complex media with simultaneous interaction of physical, chemical and biological processes. Real-time information and regular monitoring of soil mechanical composition, soil organic matter, soil nutrients and soil pH are the basis for successful crop production and mitigation of negative influence on the environment (Wetterlind, 2009). Additional attempt for precise soil management is the fact that no two soils are exactly alike, and variations occur over short distances, vertically and horizontally (Stenberg et al., 2010). Over the last two decades, many research studies have investigated visible and near infrared (VNIR) reflectance spectroscopy as non-destructive precision farming method/proximal remote sensing approach with high predictive ability to define various soil properties: total carbon and SOM content, total nitrogen content, soil pH, soil texture (Morón and Cozzolino, 2002; Udelhoven et al., 2003; McCarty and Reeves, 2006; Wetterlind et al., 2010; Fontán et al., 2011; Heinze et al., 2013; Linsler et al., 2017). VNIR hyperspectral sensing is highly sensitive to both organic and inorganic phases of the soil, making its use in the agricultural and environmental sciences particularly relevant (Viscarra Rossel et al., 2006a). The VNIR spectral region from 0.4 to 1 m contains information on soil colour, iron content and composition, soil water, and organic matter, as stated by Chabrillat et al. (2013). According to Viscarra Rossel et al. (2006b), predictions of total and organic carbon in soil, clay content and soil total nitrogen content achieve the best results, which relates with fact that clay minerals and soil organic matter represents fundamental soil compounds, and have distinctive absorption features in the VNIR spectral region. Soil pH as an important fertility regulator is reflected in complex spectral response due to its covariation with spectrally active soil properties such as organic matter and clay (Chang et al., 2001).

However, results of quantitative spectral analysis differ in dependence of measurement precision, spectral range, variability of soil properties and calibration methods used for prediction. Absorption patterns are very complex and collinear in the VNIR region, and, hence, need to be mathematically extracted from the spectra and correlated with soil properties (Stenberg et al., 2010). Multivariate algorithms commonly used in soil spectroscopy to capture the important variability in the data include partial least square regression (PLSR) as the linear method and artificial neural networks (ANN) as the non-linear method for regression type of analysis. If large numbers of independent variables are handled with a small number of samples, there is a risk of overfitting. Because each soil sample is described by several hundreds of reflectance variables, PLSR, as a “full spectrum method” seems to be a reliable method to extract the relevant part of the information from very large data matrices. The neural network gathers representative data and then invokes training algorithms to automatically learn the structure of the data. The ability of ANN to associate complicated spectral information with target attributes without any constraints for sample distribution make them ideal for describing the intricate and complex non-linear relationships which exist between soil spectral signatures and various soil properties (Kimes et al., 1998). Many authors compared and combined linear and non-linear calibration methods to increase prediction accuracy (Viscarra Rossel, 2007; Mouazen et al., 2010; Aslan-Sungur et al., 2013; Kuang et al., 2015; Morellos et al., 2016; Sorenson et al., 2017; Xu et al., 2018).

The main aim of this paper was to evaluate the ability of VNIR spectroscopy for assessment of soil properties in terms of variable mineral N fertilization and intensive crop production on field-scale level. Specific objectives included: a) discrimination of different N fertilization treatments based on soil spectra; b) prediction of soil pH, total carbon and total nitrogen content in soil using hyperspectral reflectance data; c) comparison of model performance obtained by linear and non-linear calibration methods.

Materials and methods

Experimental site and soil sampling

The study was conducted on experimental field under 20-year research on influence of mineral N fertilization on crop yield and nitrate leaching, within hydro-ameliorated cropland in Western Pannonia sub-region of Croatia (45°33´N, 16°31´E; elevation: 97.2 m). The area has a temperate continental climate, with 10.7 °C of annual mean temperature and the annual amount of rainfall of 865 mm for the reference period 1961-1990. The experiment was established as a block design of ten mineral N fertilization treatments (kg N*ha^{-1}) with uniform phosphorus (P) and potassium (K) fertilization rates (I. Control – no fertilization; II. N_0PK; III. N_{100}PK; IV. N_{150}PK; V. N_{200}PK; VI. N_{250}PK; VII. N250PK + Phospho-gypsum; VIII. N_{250}PK + Dolomite; IX. N_{300}PK; and X. Fallow), and four replication plots for each treatment (1-4). The dimension of each treatment was 30 x 130 m including blank space, and 26 x 26 m for replication plot. In order to improve soil pH, liming (S-20 mm) was applied during 2014 on all treatments except treatments II and VII. At the same year, manure application was carried out on treatments VII and VIII. The soil type of the study area is district Stagnosols (IUSS Working Group WRB, 2015). Based on the soil profile analysis, soil texture of arable topsoil was defined as loam. Precipitation water periodically stagnates on the illuvial horizon which was the reason for installing pipeline drainage system across the experiment area. Besides soil physical properties that influence water stagnation in upper layers, main factors that limit crop yield are low soil pH and very low SOM content (Table 1a. and 1b.).

Table 1a. Soil properties in 0-30 cm layer (adopted from Mesić et al., 2011)

pH/KCL	SOM (%)	Soil particles, ø mm (%)				Soil texture
		2-0.2	0.2-0.02	0.02-0.002	<0.002	
4.84	1.01	0.36	55.24	30.3	14.1	Loam

Table 1b. Soil properties in 0-30 cm layer (adopted from Mesić et al., 2011)

Porosity		Water capacity		Air capacity	
Volume (%)	Qualifier	Volume (%)	Qualifier	Volume (%)	Qualifier
43.7	Low	39.7	Medium	4	Very low

Soil sampling was performed by semi-automatic circular tractor soil probe (Patent: International Application No. PCT/HR2011/000021) after winter wheat (*Triticum aestivum* L.) harvest (13/07/2016) with total number of 200 soil samples taken at 30 cm depth (regular grid: 15x15 m), meaning 20 samples per treatment and 5 samples per repetition plot (Figure 1). Each sampling location was precisely defined (±1 cm) using GPS (Trimble GNSS R8). The point sampling scheme was circular line sampling of 0.5 m radius around the grid node representing the sampling site of the 16-samples soil composite. Samples were air-dried, milled and passed through the sieve (<2 mm), and, thus prepared for further destructive and non-destructive analysis.

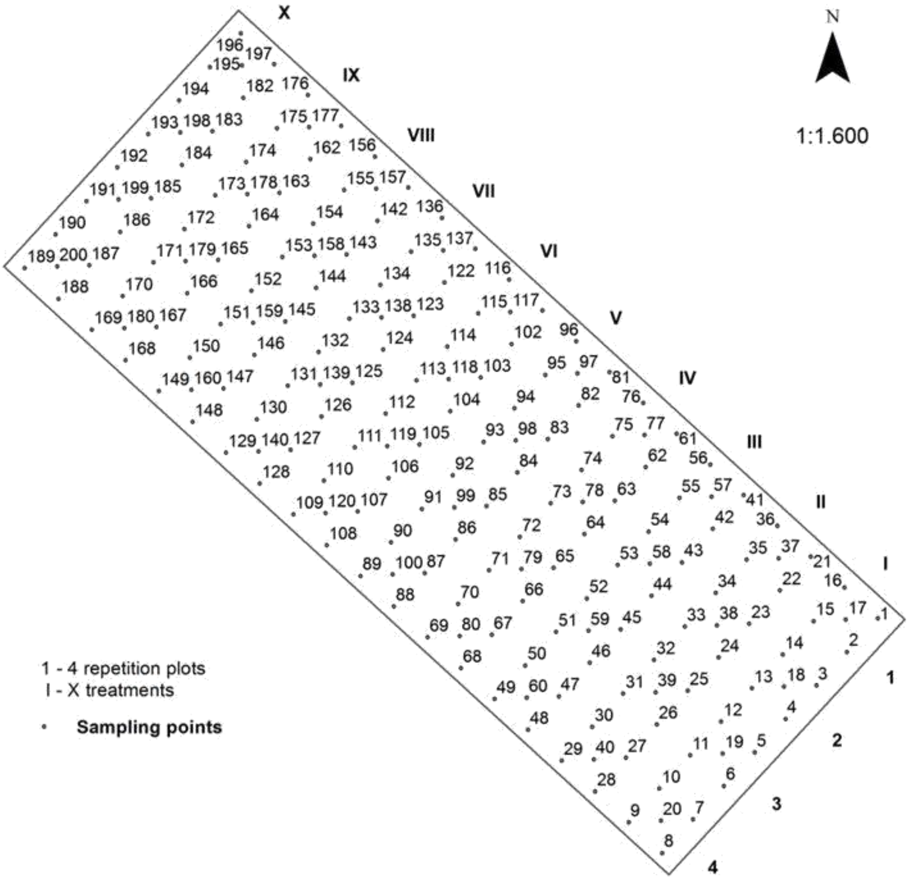


Figure 1. Scheme of the field experiment with soil sampling locations (n=200; regular grid: 15x15 m)

Spectral measurements

Proximal spectral sensing of soil samples was made in laboratory conditions using portable field spectroradiometer FieldSpec®3 (Analytical Spectral Devices Inc., 2009) with wavelength range from 350 to 1,050 nm, the sampling interval of 1.4 nm and spectral resolution of 3 nm at 700 nm. Soil samples were put on 9-cm diameter Petri dishes (borosilicate glass) forming 1.5-cm soil layer and reflectance was measured at fixed distance of 1 cm using vertically positioned hand-held fibre-optic probe with artificial illumination. Calibration panel (Spectralon®, Labsphere, Sutton, NH) measurements were taken before initial soil readings and repeated approximately every 15 minutes. Five scans of each sample were recorded at each position at an optimized integration time, with a dark current correction at every spectral measurement to minimize instrument noise and to obtain an average spectrum, used for further analysis and comparisons within and between the treatments.

Laboratory analysis

Air-dried soil samples (T<40 °C) were crumbled, sieved (<2 mm), and homogenized following ISO 11464 (2004). Soil pH was measured in a 1:2.5 (w/v) soil suspension [1 M KCl, modified ISO 10390 (2005)]. Total nitrogen content (TN [% DM; g/kg]) and total carbon content (TC [% DM; g/kg]) in soil were determined by dry combustion method according to HRN ISO 13878:2004 and HRN ISO 10694:2004, respectively.

Multivariate statistics and model performance evaluation

Spectral data as continuous input and soil properties as continuous target were used for developing prediction models. Multivariate analyses were performed using spectroscopy software Unscrambler 9.7 (CAMO Software AS, 2007) and statistical suite Statistica 8.0 (StatSoft Inc., 2007). Spectra were visually reviewed and pre-processed using ViewSpec Pro 6.2.0. (Analytical Spectral Devices Inc., 2009). Spectral bands below 430 nm were removed due to the large noise effect. Original spectra were smoothed using a Savitzky-Golay algorithm with a window size of three. Internal structure and important variability in the data were explored by principal components analysis (PCA). Factor scores acquired from the calculated principal components were used as predictor variables in selected calibration methods. Partial least square regression (PLSR) as linear calibration method and artificial neural network (ANN) as non-linear calibration method were used to build prediction models of soil pH, soil TN and TC content based on original soil reflectance data. PLSR model was calibrated using full cross validation (each observation is used as a test set to validate the predictive model). In ANN regression analysis, spectra were randomly divided into training and testing sets with proportions of 50% and 50%, respectively. The architecture of supervised back-propagation neural network was a fully connected feed-forward, with the structure consisting of input neurons which number corresponded to the number of selected PCs representing the total variation of the target spectra.

Models were validated for accuracy evaluation and predictive capability based on: correlation coefficient (r), coefficient of determination (R^2), root mean squared error (RMSE) in form of root mean squared error of calibration (RMSEC) and root mean squared error of prediction (RMSEP), and sum of square error (SSE) function for ANN learning algorithms (confidence limits of 95%). Models with the highest R^2 and the lowest RMSE were considered as the best to predict investigated soil properties.

$$RMSE = \sqrt{\frac{\sum_{i-1}^{N}(ti - yi)^2}{n}} \qquad SSE = \sum_{i-1}^{n}(yi - ti)^2$$

where y_i is the predicted value of sample *i*; t_i is the observed value of sample *i*; *n* is the total number of samples.

Results and discussion

Soil properties

Figure 2a-c represents average values of soil pH, TC (%) and TN (%) in soil according to ten N fertilization treatments, measured with standard laboratory analysis. These are results of 20-year intensive mineral N fertilization on soil characterized by heavy texture and low soil pH. Soil TC and TN content increased with increasing fertilizer amounts and show almost collinear trend. Regarding very low average soil pH indicating acid soil, and assumption that mineral carbon is not present in investigated soil, TC can be equalized to soil organic C. As stated by Stenberg et al. (2010), N content in soil is almost as related to the organic matter content as organic C, as the absolute majority of the N is organic and typically comprises about 1/10 of the organic C. Correlation matrix between soil properties confirmed this relation through full significant correlation for TC and TN (r=0.96) (Table 2). Due to both reduction processes in illuvial horizon caused by water stagnation and long-term mineral N fertilization, soil pH had decreasing trend up to 200 kg N*ha^{-1}, whereupon rise to 5.27 at the Fallow treatment. Significant strong negative correlation was calculated between soil pH and both TC and TN content. After years of mineral fertilization and progressive soil acidification, the formation of acid humus could explain this specific relation.

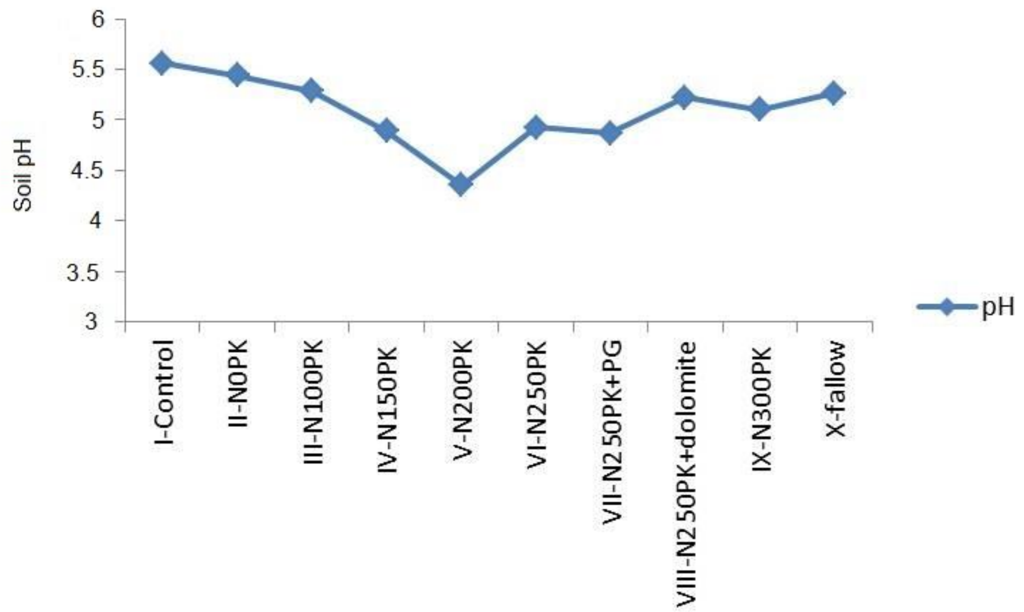


Figure 2a. Mean soil pH between different N fertilizer treatments

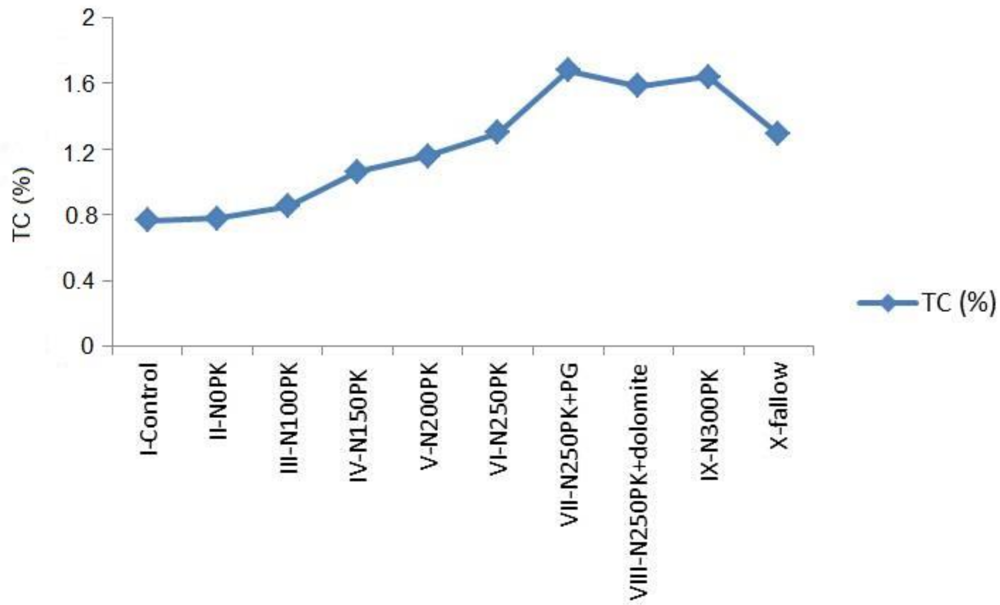


Figure 2b. Mean total carbon content (TC, %) in soil between different N fertilizer treatments

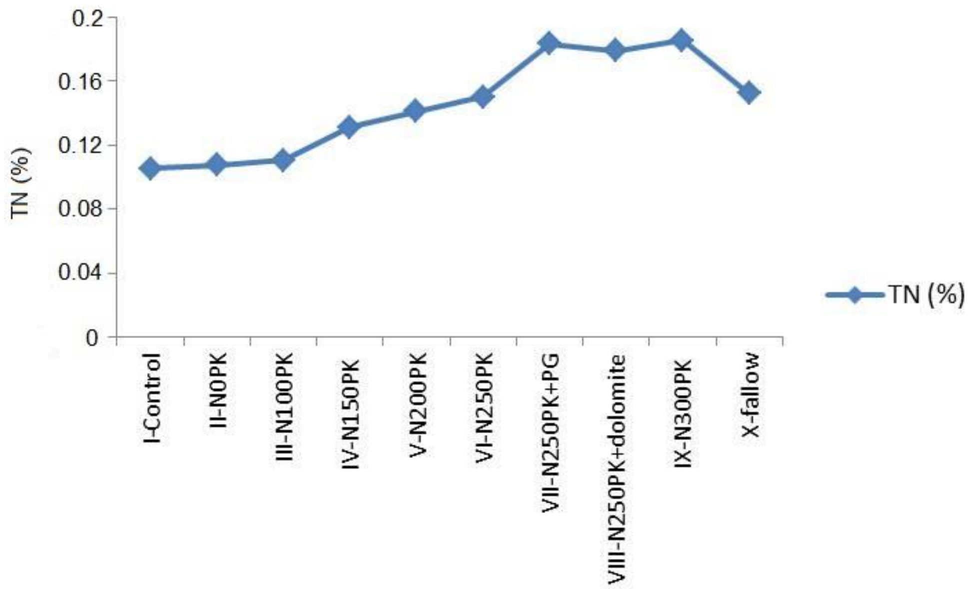


Figure 2c. Mean total nitrogen content (TN, %) in soil between different N fertilizer treatments

Table 2. Descriptive statistics and correlation matrix between soil properties (n=200)

Variable	Means	Standard deviation	Coefficient of correlation (r)		
			TC (%)	TN (%)	pH
TC (%)	1.205	0.417	1	0.96	-0.52
TN (%)	0.144	0.038	0.96	1	-0.53
pH	5.01	0.98	-0.52	-0.53	1

Correlations are significant at $P<0.05$.

Treatment effect on soil reflectance properties

Figure 3 shows average soil reflectance spectra and its first derivative for ten fertilization treatments. The reflectance curves exhibited the typical pattern of soil spectra, with the reflectance generally lower in the visible range (350–700 nm) and higher in the near infrared region (700–1,050 nm). Different N fertilization treatments indicated very collinear soil spectral response, but with certain variations of reflectance intensity. Raw reflectance showed increasing curve from visible range towards higher wavelengths in NIR region where reflectance factor reached value of 0.45. However, absorption is weaker around 450 nm and 850 nm, which can be explained by removing of clay and free iron oxides in the eluvial process, as stated by Šestak et al. (2018). In the spectral range of 350-1050 nm, soil reflectance achieved common features (McCoy, 2005): less organic carbon content – higher reflectance; more organic carbon content - lower reflectance. Two groups of soil spectra can be distinguished according to fertilization treatments: 1) I. Control; II. N_0PK; $N_{100}PK$; VIII. $N_{250}PK$ + Dolomite; X. Fallow; and 2) IV. $N_{150}PK$; V. $N_{200}PK$; VI. $N_{250}PK$; VII. $N_{250}PK$ + Phospho-gypsum; IX. $N_{300}PK$. The first group was characterized by lower TC content, but higher soil pH influenced on soil colour as captured with VNIR reflectance in the sense of darker tone, non-acid humus formation and no bleaching traces. Water stagnation induced reduction processes on treatments from second group, which revealed lower soil pH together with the effect of long-term N fertilization. However, lighter soil colour caused by bleaching processes masked the fact that these samples had higher TC content, in form of acid humus. According to the presence of higher silt and fine sand content in the topsoil, there is an assumption that soil particle size had the effect on stronger soil spectral reflectance (Dematte et al., 2004).

DOI: /10.5513/JCEA01/20.1.2158

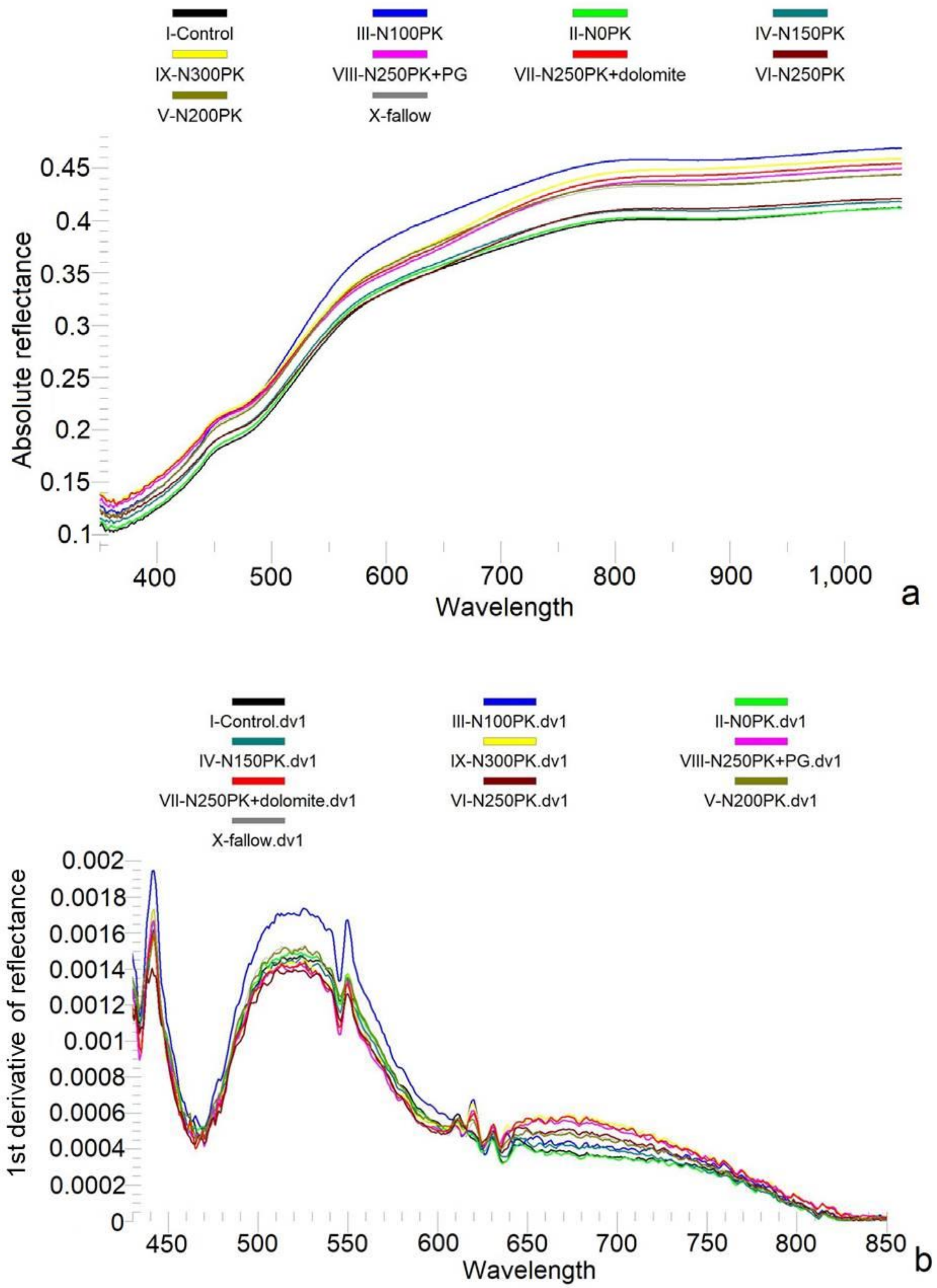
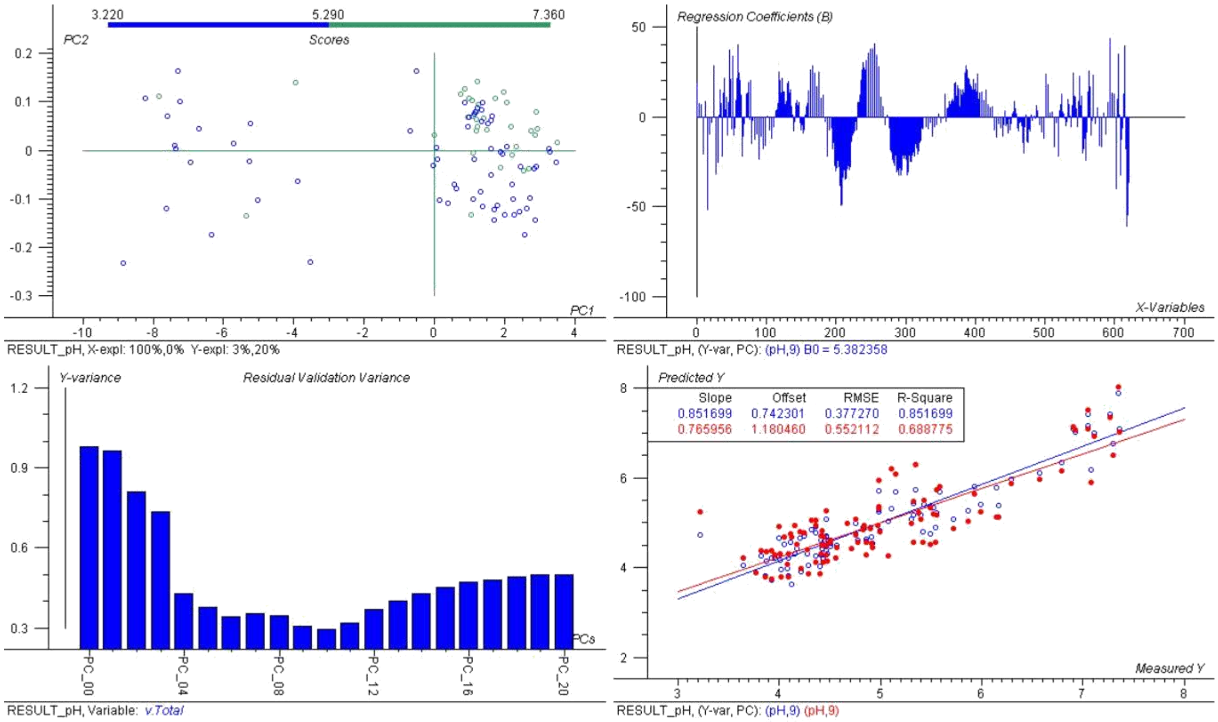
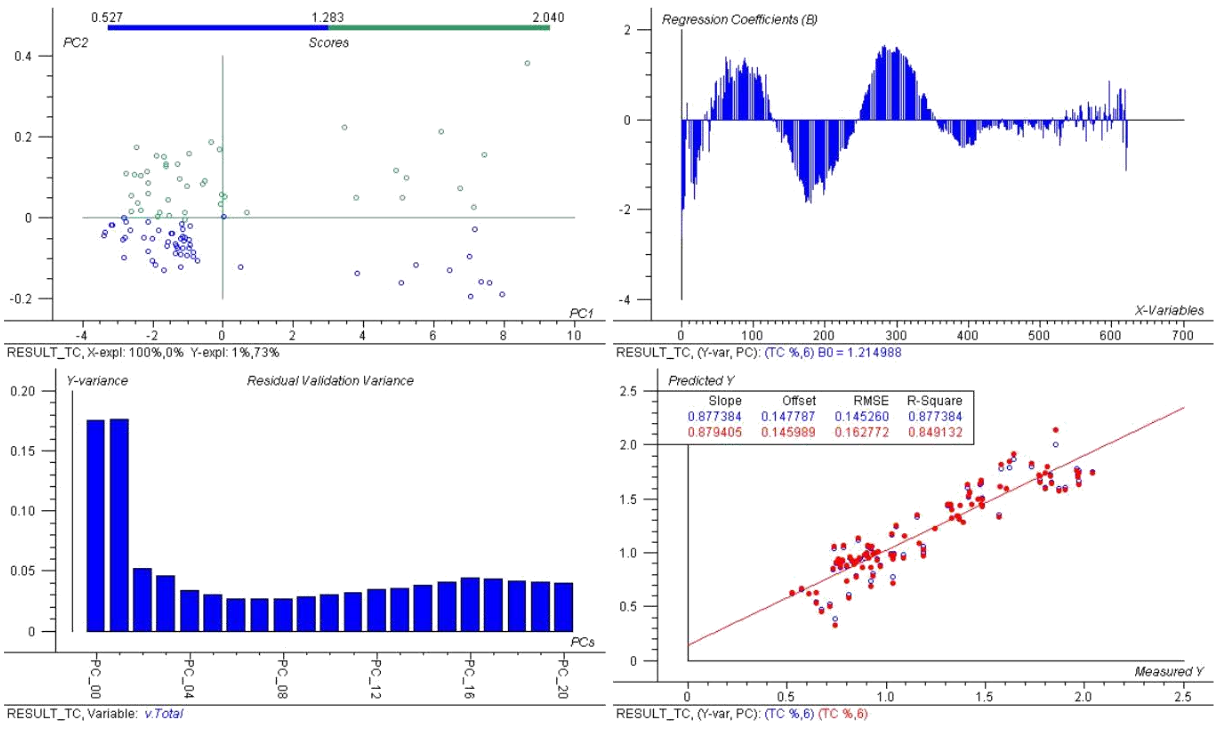


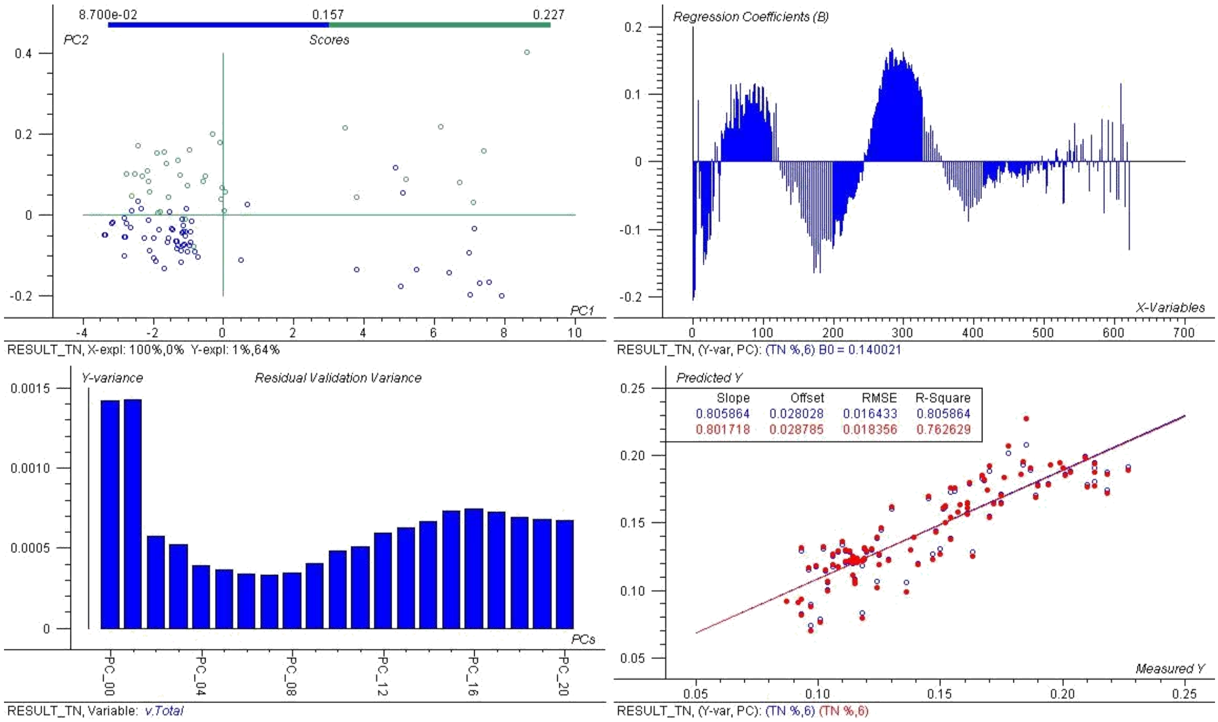
Figure 3. Difference in average absolute soil reflectance (a) and average first derivative of soil reflectance (b) at ten fertilization treatments

Performance of PLSR models

Partial least square regression (PLSR) and artificial neural networks (ANN) were used to build prediction models of soil pH, TC and TN content in soil based on VNIR spectra. Figure 4 represents results of the PLSR model calibrated to estimate soil pH (upper figure), TC content (medium figure), and TN content (bottom figure) using original soil reflectance and reference sample data. As seen from the principal component (PC) score plot, spectral data successfully delineated between higher and lower values of investigated soil properties. Variation in soil pH as a covariate of other fertility indicators followed the similar structure in PC space. The PLSR prediction model for soil pH, TC and TN content revealed very strong to complete correlation and low root mean squared error between predicted and measured values for the calibration and validation dataset, respectively (TC, %: R^2=0.88 and R^2=0.85, RMSEC=0.145 and RMSEP=0.163; TN, %: R^2=0.81 and R^2=0.76, RMSEC=0.016 and RMSEP=0.018; soil pH: R^2=0.85 and R^2=0.69, RMSEC=0.38 and RMSEP=0.55), as summarized in Table 3. Calculated parameters are in line with local calibrations for soil pH, TN and TC in soil reported by Wetterlind et al. (2010) (R^2=0.65-0.85, RMSEP=0.1-0.15; R^2=0.82-0.85, RMSEP=0.016-0.024%; R^2=0.89-0.92; RMSEP=0.16-0.17%, respectively). Kuang and Mouazen (2011) also evaluated the ability of VNIR spectroscopy (450–2,450 nm) to predict TC, TN and organic C in fresh soil samples on three European farms. They reported calibrations with R^2 of 0.85–0.93 for the cross-validation. In this case, water absorption was observed utilizing a wider spectral range. According to Haiqing Yang (2011) who measured VNIR reflectance on air-dried samples at the farm scale, PLSR (cross validation) on original spectra gave results comparable to this paper with R^2 of 0.81 and RMSEP of 0.025 for TN content (%), and R^2 of 0.82 and RMSEP of 0.232 for organic C content in soil. Conforti et al. (2018) used VNIR spectroscopy coupled with PLSR for predicting SOC, TN, pH, which yielded very promising results (R^2 of 0.88, 0.82, 0.7, and RMSEP of 0.79%, 0.06%, 0.15, respectively). As seen from the regression coefficients plot (Figure 4), visible wavelengths (450-550 nm) with red to red edge region (670-760-800 nm) mostly contributed to variation in the data, indicating primarily effect of soil color (factors: soil organic carbon, soil texture) on soil spectra. These results are consistent with Peón et al. (2017), who used airborne hyperspectral data to estimate soil organic carbon and found an absorption feature in the red region of the spectrum, with the maximum absolute correlation at the wavelengths at 610 and 679–681 nm, as relevant for TOC/OC predictions. Lopez-Granados et al. (2005) found blue spectral region highly correlated with soil organic matter and soil pH. Mouazen et al. (2010) distinguished two peaks in visible range at about 490 and 640 associated with the blue region around 450 nm and the red region around 680 nm. According to Conforti et al. (2018), the best correlation coefficients between soil organic C and TN with soil spectra were found in the spectral domain between 500 and 800 nm with the strongest one at 610 nm and 600 nm, respectively.


Scores
PC1
PC2
RESULT_pH, X-expl: 100%,0% Y-expl: 3%,20%
Regression Coefficients (B)
X-Variables
RESULT_pH, (Y-var, PC): (pH,9) B0 = 5.382358
Y-variance
Residual Validation Variance
PCs
RESULT_pH, Variable: v.Total
Predicted Y
Slope Offset RMSE R-Square
0.851699 0.742301 0.377270 0.851699
0.765956 1.180460 0.552112 0.688775
Measured Y
RESULT_pH, (Y-var, PC): (pH,9) (pH,9)


Scores
PC1
PC2
RESULT_TC, X-expl: 100%,0% Y-expl: 1%,73%
Regression Coefficients (B)
X-Variables
RESULT_TC, (Y-var, PC): (TC %,6) B0 = 1.214988
Y-variance
Residual Validation Variance
PCs
RESULT_TC, Variable: v.Total
Predicted Y
Slope Offset RMSE R-Square
0.877384 0.147787 0.145260 0.877384
0.879405 0.145989 0.162772 0.849132
Measured Y
RESULT_TC, (Y-var, PC): (TC %,6) (TC %,6)



Content based on soil reflectance data (n=200), □ calibration; □ validation.

Figure 4. Scatter plots for results of the PLSR model showing relationship between predicted and observed soil pH, total carbon (TC, %) and total nitrogen (TN, %) content (from top to bottom, respectively)

Table 3. Summary of PLSR and ANN prediction models

Model	NPC	Calibration		Validation	
		R^2	RMSEC	R^2	RMSEP
			TC (%)		
PLSR	6	0.88	0.145	0.85	0.163
ANN	14	0.96	0.067	0.88	0.108
			TN (%)		
PLSR	6	0.81	0.016	0.76	0.018
ANN	14	0.96	0.006	0.86	0.012
			pH		
PLSR	9	0.85	0.38	0.69	0.55
ANN	14	0.8	0.31	0.74	0.42

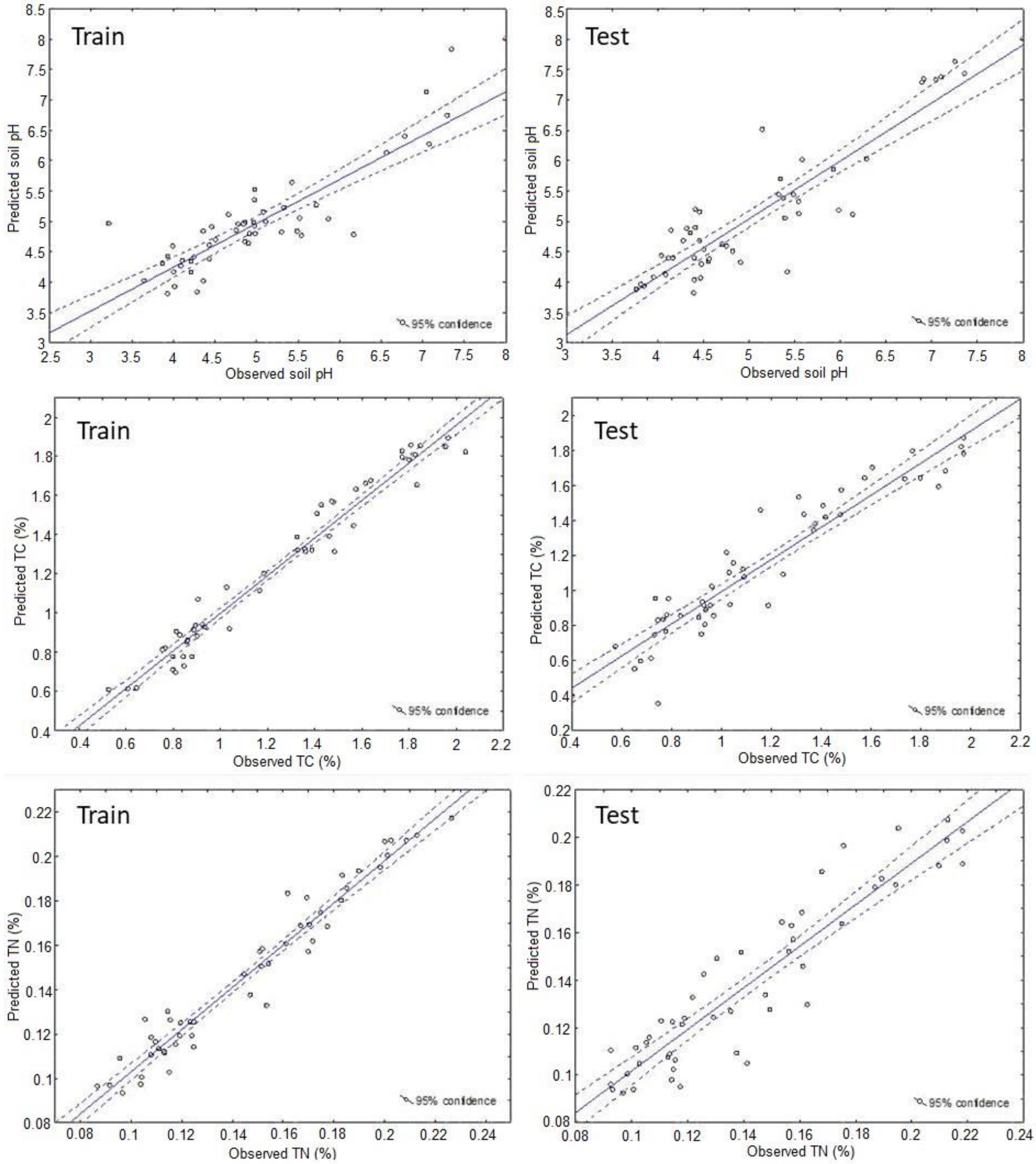
NPC - optimal number of principal components; R^2 - coefficient of determination; RMSEC - root mean square error of calibration; RMSEP - root mean square error of prediction.

Performance of ANN models

To capture complex linear relations between spectral data and soil properties, machine learning algorithms in form of a robust back propagation neural network (see ANN) were invoked to learn the structure of data and calculate variability explained by soil VNIR reflectance. Neural network structure was MLP (Multilayer perceptron) with 1 hidden layer and 14 input PCs, and BFGS iterative technique. Predicted vs. observed soil pH, TC and TN content relationship for train/calibration (left score plot) and test/validation (right score plot) dataset explained using ANN regression were found to have very strong to complete correlation (Figure 5, Table 3), which indicated good learning performance. Cumulative results of ANN model for soil pH, TC and TN content between predicted and measured values for the calibration and validation dataset, respectively, are shown in Table 3 (TC, %: R^2=0.96 and R^2=0.88, RMSEC=0.067 and RMSEP=0.108; TN, %: R^2=0.96 and R^2=0.86, RMSEC=0.006 and RMSEP=0.012; soil pH: R^2=0.8 and R^2=0.74, RMSEC=0.31 and RMSEP=0.42).

Although both calibration methods yielded good predictions, ANN models were more efficient in capturing the complex link between selected soil properties and soil reflectance spectra than PLSR. According to Mouazen et al. (2010) who compared PLSR, principal component regression and neural networks, back propagation neural network model outperformed PCR and PLSR for soil organic C content (validation R^2=0.84). Similar conclusion gave Kuang et al. (2015) who recommend ANN as calibration method for on-line VNIR prediction of organic carbon, pH and clay content, while Morellos et al. (2016) found machine learning methods to perform better than the multivariate regression methods in prediction of organic carbon and TN in fresh samples.

All observed studies are in close correspondence with results of this research which achieved reliable performance although utilizing only spectral range of 430-1,050 nm. Developed models represent soil-, field- and farm- specific calibrations, and, hence, valuable contribution to the soil spectral databases. Very close relationship between soil TC (mostly organic in this case) and TN, as spectrally active soil constituents, and strong covariation with soil pH revealed spectral response mostly in the visible part of the spectrum which participated in building model predictions for stated soil properties.



Input neurons are PC scores of the original reflectance (dash lines: P<0.05).

Figure 5. Comparison of predicted and observed soil pH, total carbon (TC, %) and total nitrogen (TN, %) content using ANN regression model for train set (50%) and test set (50%), respectively

Conclusions

The research findings confirmed the high applicability of laboratory soil VNIR spectroscopy as a non-destructive and cost-effective precision farming tool for monitoring changes in soil properties, particularly in the assessment of soil pH, TC and TN soil content, under the conditions of intensive crop production.

The PLSR prediction model for soil pH, TC and TN content revealed very strong to complete correlation and low root mean squared error between predicted and measured values for the calibration and validation dataset, respectively (TC, %: R^2=0.88 and R^2=0.85, RMSEC=0.145 and RMSEP=0.163; TN, %: R^2=0.81 and R^2=0.76, RMSEC=0.016 and RMSEP=0.018; soil pH: R^2=0.85 and R^2=0.69, RMSEC=0.38 and RMSEP=0.55).

Results of ANN model for soil pH, TC and TN content between predicted and measured values for the both datasets showed very strong to complete correlation, respectively (TC, %: R^2=0.96 and R^2=0.88, RMSEC=0.067 and RMSEP=0.108; TN, %: R^2=0.96 and R^2=0.86, RMSEC=0.006 and RMSEP=0.012; soil pH: R^2=0.8 and R^2=0.74, RMSEC=0.31 and RMSEP=0.42).

ANN models were more efficient in capturing the complex link between selected soil properties and soil reflectance spectra than PLSR. Red part of the spectrum with red edge region was identified as the zone of major contribution for soil TC and TN predictions.

Soil pH as a covariate of other fertility indicators (r=-0.52 and r=-0.53 for TC and TN content, respectively) dictated reflectance response curves of TC and TN content. Areas with higher SOM content correlated with low-pH zones probably due to the presence of organic acids, resulting in higher soil reflectance influenced by bleaching traits as well. Lower reflection was observed at treatments with high SOM content and high soil pH.

VNIR calibrations defined in this research should help to support site-specific soil survey in agriculture as addition to standard laboratory analysis. Moreover, applying hyperspectral ranges in shortwave and midwave infrared spectrum would enhance knowledge on optical soil properties, and enable integration with airborne sensors.

References

Analytical Spectral Devices Inc. (2009) ViewSpec Pro 4.07 Software. Boulder: Analytical Spectral Devices Inc.

Aslan-Sungur, G., Evrendilek, F., Karakaya, N., Gungor, K., Kilic, S. (2013) Integrating ATR FTIR and data-driven models to predict total soil carbon and nitrogen towards sustainable watershed management. Research Journal of Chemistry and Environment, 17 (6), 5-11.

CAMO Software AS (2007) UNSCRAMBLER 9.7. Spectroscopy Software Suite. Oslo: CAMO Software AS.

Chabrillat, S., Ben-Dor, E., Viscarra Rossel, R.A., Demattê, J.A.M. (2013) Editorial: Quantitative soil spectroscopy. Applied and Environmental Soil Science, 1-3. DOI: http://dx.doi.org/10.1155/2013/616578

Chang, C.W., Laird, D.A., Mausbach, M.J., Hurburgh, C.R. (2001) Near-infrared reflectance spectroscopy - principal components regression analyses of soil properties. Soil Science Society of America Journal, 65 (2), 480–490. DOI: https://dx.doi.org/10.2136/sssaj2001.652480x

Conforti, M., Matteucci, G., Buttafuoco, G. (2018) Using laboratory Vis-NIR spectroscopy for monitoring some forest soil properties. Journal of Soils and Sediments, 18 (3), 1009–1019. DOI: https://doi.org/10.1007/s11368-017-1766-5

Dematte, J.A.M., Campos, R.C., Alves, M.C., Fiorio, P.R., Nanni, M.R. (2004) Visible NIR- reflectance: a new approach on soil evaluation. Geoderma, 121 (1-2), 95-112. DOI: https://doi.org/10.1016/j.geoderma.2003.09.012

Fontán, J.M., López-Bellido, L., García-Olmo, López-Bellido, R.J. (2011) Soil carbon determination in a Mediterranean vertisol by visible and near infrared reflectance spectroscopy. Journal of Near Infrared Spectroscopy, 19 (4), 253–263. DOI: https://doi.org/10.1255/jnirs.936

Heinze, S., Vohland, M., Joergensen, R.G., Ludwig, B. (2013) Usefulness of near-infrared spectroscopy for the prediction of chemical and biological soil properties in different long-term experiments. Journal of Plant Nutrition and Soil Science, 176 (4), 520-528. DOI: https://doi.org/10.1002/jpln.201200483

International Organization for Standardization (2004) ISO 10694: Soil quality - determination of organic and total carbon after dry combustion (elementary analysis). Geneva: International Organization for Standardization.

International Organization for Standardization (2004) ISO 11464: Soil quality - pretreatment of samples for physico-chemical analyses. Geneva: International Organization for Standardization.

International Organization for Standardization (2004) ISO 13878: Soil quality - determination of total nitrogen content by dry combustion (elementary analysis). Geneva: International Organization for Standardization.

International Organization for Standardization (2005) ISO 10390: Soil quality - determination of pH. Geneva: International Organization for Standardization.

IUSS Working Group WRB (2015) World Reference Base for Soil Resources. International soil classification system for naming soils and creating legends for soil maps. World soil resources reports no. 106. Rome: FAO. Available at: http://www.fao.org/3/a-i3794e.pdf

Kimes, D.S., Nelson, R.F., Manry, M.T., Fung, A.K. (1998) Attributes of neural networks for extracting continuous vegetation variables from optical and radar measurements. International Journal of Remote Sensing, 19 (14), 2639–2663. DOI: https://doi.org/10.1080/014311698214433

Kuang, B., Mouazen, A.M. (2011) Calibration of visible and near infrared spectroscopy for soil analysis at the field scale on three European farms. European Journal of Soil Science, 62 (4), 629–636. DOI: https://doi.org/10.1111/j.1365-2389.2011.01358.x

Kuang, B., Tekin, Y., Mouazen, A.M. (2015) Comparison between artificial neural network and partial least squares for on-line visible and near infrared spectroscopy measurement of soil organic carbon, pH and clay content. Soil and Tillage Research, 146 (B), 243–252. DOI: https://doi.org/10.1016/j.still.2014.11.002

Linsler, D., Sawallisch, A., Höper, H., Schmidt, H., Vohland, M., Ludwig, B. (2017) Near-infrared spectroscopy for determination of soil organic C, microbial biomass C and C and N fractions in a heterogeneous sample of German arable surface soils. Archives of Agronomy and Soil Science, 63 (11), 1499–1509. DOI: https://doi.org/10.1080/03650340.2017.1292030

Lopez-Granados, F., Jurado-Exposito, M., Pena-Barragan, J.M., Garcia-Torres, L. (2005) Using geostatistical and remote sensing approaches for mapping soil properties. European Journal of Agronomy, 23 (3), 279-289. DOI: https://doi.org/10.1016/j.eja.2004.12.003

McCarty, G.W., Reeves, J.B. (2006) Comparison of near infrared and mid infrared diffuse reflectance spectroscopy for field-scale measurement of soil fertility parameters. Soil Science, 171 (2), 94–102. DOI: https://doi.org/10.1097/01.ss.0000187377.84391.54

McCoy, R.M. (2005) Field methods in remote sensing. New York: The Guilford Press.

Mesić, M., Zgorelec, Ž., Šestak, I., Jurišić, A. (2011) Nitrogen fertilization acceptable for environment (scientific report for 2010). Zagreb: University of Zagreb, Faculty of Agriculture.

Morellos, A., Pantazi, X.-E., Moshou, D., Alexandridis, T., Whetton, R., Tziotzios, G., Wiebensohn, J., Bill, R., Mouazen, A.M. (2016) Machine learning based prediction of soil total nitrogen, organic carbon and moisture content by using VIS-NIR spectroscopy. Biosystems Engineering, 152, 104-116. DOI: https://doi.org/10.1016/j.biosystemseng.2016.04.018

Morón, A., Cozzolino, D. (2002) Application of near Infrared Reflectance Spectroscopy for the Analysis of Organic C, Total N and pH in Soils of Uruguay. Journal of Near Infrared Spectroscopy, 10 (3), 215-221.

Mouazen, A.M., Kuang, B., De Baerdemaeker, J., Ramon, H. (2010) Comparison among principal component, partial least squares and back propagation neural network analyses for accuracy of measurement of selected soil properties with visible and near infrared spectroscopy. Geoderma, 158 (1-2), 23–31. DOI: https://doi.org/10.1016/j.geoderma.2010.03.001

Peón, J., Recondo, C., Fernández, S., Calleja, J.F., De Miguel, E., Carretero, L. (2017) Prediction of topsoil organic carbon using airborne and satellite hyperspectral imagery remote sensing, 9 (12), 1211. DOI: https://doi.org/10.3390/rs9121211

Sorenson, P.T., Small, C., Tappert, M.C., Quideau, S.A., Drozdowski, B., Underwood, A., Janz, A. (2017) Monitoring organic carbon, total nitrogen, and pH for reclaimed soils using field reflectance spectroscopy. Canadian Journal of Soil Science, 97 (2), 241–248. DOI: https://doi.org/10.1139/cjss-2016-0116

StatSoft Inc. (2007) STATISTICA 8.0. Data analysis software system. Tulsa, Oklahoma: StatSoft Inc.

Stenberg, B., Viscarra Rossel, R.A., Mouazen, A.M., Wetterlind, J. (2010) Visible and near infrared spectroscopy in soil science. Advances in Agronomy, 107, 163-215. DOI: https://doi.org/10.1016/S0065-2113(10)07005-7

Šestak, I., Mesić, M., Zgorelec, Ž., Perčin, A., Stupnišek, I. (2018) Visible and near infrared reflectance spectroscopy for field-scale assessment of Stagnosols properties. Plant, Soil and Environment, 64 (6), 276–282. DOI: https://doi.org/10.17221/220/2018-PSE

Udelhoven, T., Emmerling, C., Jarmer, T. (2003) Quantitative analysis of soil chemical properties with diffuse reflectance spectrometry and partial least-square regression: a feasibility study. Plant and soil, 251 (2), 319-329.

Viscarra Rossel, R.A., Minasny, B., Roudier, P., McBratney, A.B. (2006a) Colour space models for soil science. Geoderma, 133 (3), 320–337. DOI: https://doi.org/10.1016/j.geoderma.2005.07.017

Viscarra Rossel, R.A., Walvoort, D.J.J., McBratney, A.B., Janik, L.J., Skjemstad, J.O. (2006b) Visible, near infrared, mid infrared or combined diffuse reflectance spectroscopy for simultaneous assessment of various soil properties. Geoderma, 131 (1-2), 59–75. DOI: https://doi.org/10.1016/j.geoderma.2005.03.007

Viscarra Rossel, R.A. (2007) Robust modelling of soil diffuse reflectance spectra by „bagging-partial least squares regression". Journal of Near Infrared Spectroscopy, 15 (1), 39–47. DOI: https://doi.org/10.1255/jnirs.694

Wetterlind, J. (2009) Improved farm soil mapping using near infrared reflection spectroscopy. Doctoral thesis. Uppsala: Sveriges lantbruksuniv.

Wetterlind, J., Stenberg, B., Söderström, M. (2010) Increased sample point density in farm soil mapping by local calibration of visible and near infrared prediction models. Geoderma, 156 (3-4), 152–160. DOI: https://doi.org/10.1016/j.geoderma.2010.02.012

Xu, S., Zhao, Y., Wang, M., Shi, M. (2018) Comparison of multivariate methods for estimating selected soil properties from intact soil cores of paddy fields by Vis-NIR spectroscopy. Geoderma, 310, 29-43. DOI: https://doi.org/10.1016/j.geoderma.2017.09.013

Yang, H. (2011) Spectroscopic calibration for soil N and C measurement at a farm scale. Procedia Environmental Sciences, 10 (A), 672 – 677. DOI: https://doi.org/10.1016/j.proenv.2011.09.108